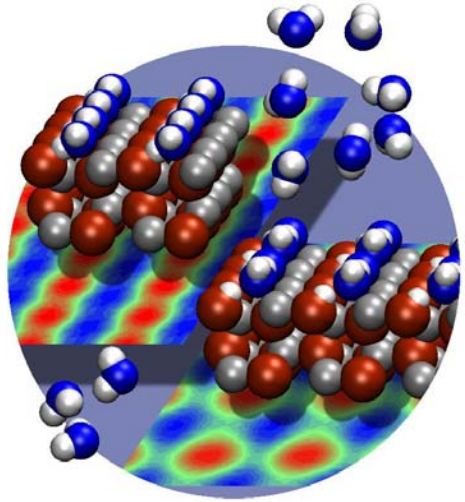
Nanoscale Surface Investigations of Semiconducting Metal Oxides

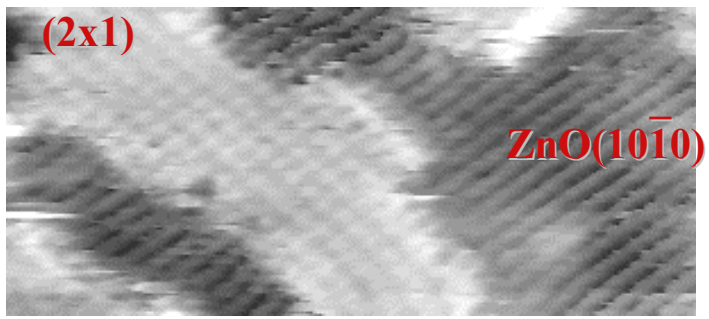
Ulrike Diebold, Tulane University

Award # (CHE-0109804)

The formation of partially dissociated ordered superstructures upon covering defect-free surfaces by water molecules is advanced as an intriguing, but controversial intermediate scenario between complete wetting and full dissociation. Conclusive evidence is given that such a phenomenon is encountered for H_2O on the perfect ZnO(1010) surface. At monolayer coverage, every second water molecule is found to dissociate. A favorable hydrogen-bonding interaction with a neighboring water molecule leads to a low activation barrier; no defects or impurities are invoked. This process leads to a (2 x 1) superlattice with long-range order which is stable from well below room temperature up to temperatures close to the boiling point of liquid water.



15 x 8 nm^2



STM image of an ordered 2x1 water cluster

B. Meyer, D. Marx, O. Dulub, U. Diebold, M. Kunat, D. Langenberg, C. Wöll, "Partial Dissociation Water on the Surface of Zinc Oxide"Angewandte Chemie, Int. Edition, *in press*

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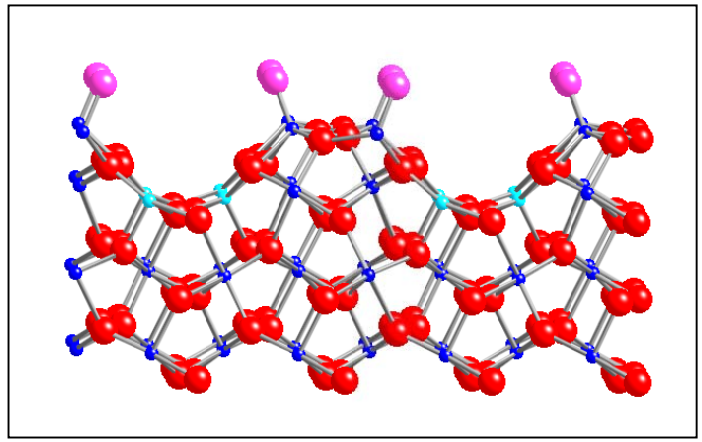
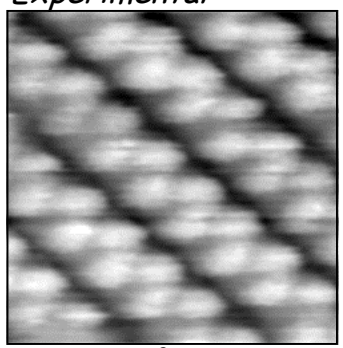
Titanium dioxide is a promising photocatalyst for the remediation of pollutants and the photoelectrochemical conversion of solar energy. For certain photocatalytic oxidation reactions the {011} facets of rutile TiO_2 are particularly active. It has been speculated that a special atomic configuration on TiO_2(011) alters either the efficiency with which photogenerated carriers are trapped at the surface, or the rate at which they are transferred at the solid-liquid interface. We wanted to find out what this special configuration might be. In a combined experimental and theoretical study we show that the TiO_2(011) surface exhibits a (2 x 1) reconstruction and is distinct from other TiO_2 surfaces by the presence of one-fold coordinated (titanyl) oxygen atoms. We suggest that these species play a special role in the enhanced photocatalytic activity of the TiO_2 (011) surface.

Model



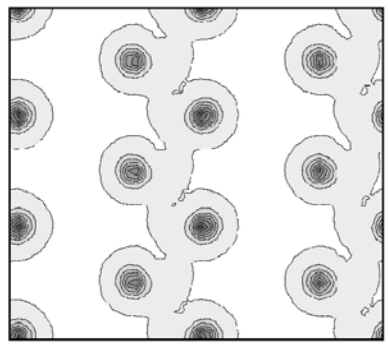
Empty-states STM images of TiO_2(011) -(1x2):

Experimental



34 Å, +1.7 V, 0.97 nA

Calculated



T.J. Beck, A. Klust, M. Batzill, U. Diebold, Cristiana di Valentin, Annabella Selloni
"Surface Structure of TiO_2(011)-(1x2)" Physical Review Letters 93 (3) (2004) 036104